Benzenesulfonic acid, 3-hydrazino-138-30-7 | DTXSID8059681

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 5.98e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.76e-01

Confidence level: 5.96e-01

Nearest Neighbors from the Training Set

Image not found

1H-Imidazole-5-sulfonic acid

Measured: 1.35 Predicted: 7.40e-01

Image not found

1H-Imidazole-2-sulfonic acid

Measured: 8.44e-01 Predicted: 7.41e-01

Image not found

Benzenesulfonic acid, 3-

hydrazino-

Measured: 1.49e-01 Predicted: 5.98e-01

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Taurocyamine
Measured: 2.33e-01
Predicted: 3.13e-01